

# ASSESSMENT OF COAL REACTIVITY DURING PREHEATING BY THE RELATIONSHIPS BETWEEN STRUCTURAL AND PLASTIC PROPERTIES. CHEMOMETRIC ANALYSES.

N. Pieri, L. Quoniam, J. Kister, Laboratoire GOAE, Aix-Marseille III University, Case 561,  
13397 Marseille Cedex 20, France,

M. A. Diez, R. Alvarez, J.J. Pis, Instituto Nacional del Carbón (INCAR), CSIC, Apartado 73,  
33080 Oviedo, España.

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## ABSTRACT

Relatively little attention has been given to determine the coal structural changes induced by industrial preheating process. In this work, a series of ten coking coals was characterized, before and after industrial preheating, by FTIR and Synchronous UV Fluorescence (SF) spectroscopies and by petrography and plastic properties (e.g. mean Reflectance and Gieseler maximum fluidity, Fm). Specific structural indices derived from FTIR and SF data were defined and used in Principal Component Analysis to determine the effects of coal preheating on structural changes and to classify coals on the basis of plastic and petrography characteristics. Predicted models of plastic and petrography properties were established from FTIR and SF indices using Multivariate Linear Regression. For example, Gieseler Fm and volatile matter content, two main parameters for coal blending, can be estimated from the FTIR and SF indices for wet and preheated coals. Thus a better insight into reactivity of coking coals and a valuable estimation of their properties can be accounted.

## INTRODUCTION

Recently, reserves of good coking coals have become less available and comparatively more expensive. Resources are extended by using coal blends with different coking properties and/or selective additives. Coal preheating technology has emerged as a technique to overcome some of these problems. This technology, preheating of coal at about 200°C in an inert atmosphere, in combination with the dry cooling of the resulting coke, is now incorporated into the operation of the Jumbo Coking Reactor (JRC, European Eureka Research Project)<sup>1</sup>.

Most studies of preheating have focused on advantages in terms of technological improvements to coke quality and productivity, together with widening the range of coals suitable for coking compared to conventional wet gravity charging<sup>2</sup>. Industrial preheating produces a decrease in the volatile content of the preheated coal compared to the original coal due to a devolatilization of the coal particles, accompanied by coal particle pore formation<sup>3</sup>. However, relatively little attention has been given to determining the structural changes induced in coals by industrial preheating process. These chemical transformations can be accurately evidenced by routine or more sophisticated analytical techniques.

The small molecules, trapped in the pores of coal macromolecular structure, have been defined as the mobile components in coals, and they are extractable using organic solvents<sup>4-5</sup>. Brown and Waters<sup>6</sup> have shown that the mobile component extracted with CHCl<sub>3</sub> plays an important role in the development of coking ability. Previous studies have shown that UV Synchronous Fluorescence (SF) spectroscopy is interesting for qualitative and quantitative analysis of aromatic compounds present in the extractable organic matter<sup>7-8</sup>. Furthermore, a new ranking parameter for coals which present a large range of petrographic and chemical characteristics has been established from SF data<sup>9</sup>. Despite of the non applicability of this ranking parameter for coals comprised in a similar range, this technique can be used to determine the structural changes related to aromatics in the extractable phase<sup>10-12</sup>. Moreover, structural information of coal residue can be assessed by Fourier transformed infrared (FTIR) spectroscopy<sup>13-15</sup>.

It may be assumed that the nature and the extent of the chemical transformations associated with the preheating process depend on the initial composition of coal i.e. its origin and its rank. In order to evidence the effects of initial composition on the rank and the coking properties of coals, a coal series was preheated and analyzed by FTIR and SF spectroscopies before and after preheating. This paper presents the results of the analysis of the different coals and emphasizes the effect of origin-preheating pair on the plastic behavior of coals, using chemometric analyses.

## EXPERIMENTAL

A series of international coking coals (H) was selected for the industrial coal preheating process (Table 1). Coal preheating was carried out in the 2t/h INCAR pilot plant -Precarbon process- at 210 ± 10 °C under an inert atmosphere<sup>16</sup>. A coal sampling was performed : the wet coal before

being charged into the preheating pilot plant (H) and the preheated coal in the closed conveyor before entering to the coke-oven (P).

The particle fractions of wet and preheated coals ( $< 150\mu\text{m}$ ) were ultrasonically extracted with  $\text{CHCl}_3$  (100 mg coal / 30 ml solvent) for 45 min. Extract yields were about 2 wt%. After removing solvent, extracts were dissolved in THF (10 mg/l) for SF measurements. SF spectra were obtained at a fixed excitation and emission wavelength interval of 23 nm, excitation and emission beams being kept at a width of 5 nm and a scanning rate of 200 nm/s, in the 200-600 nm range. Selected indices derived from SF data using the integrated area (A) of different spectral bands are described in Table 2.

The extraction residues were analyzed by FTIR spectroscopy using KBr standard pellets (1:150 coal residue to KBr ratio). Each spectrum resulted from the accumulation of 128 scans, recorded with a spectral resolution of  $4\text{ cm}^{-1}$  in the  $4000\text{-}400\text{ cm}^{-1}$  spectral domain, was normalized to 1 mg of sample. Mineral matter interferences were eliminated by subtracting the corresponding spectrum of the low-temperature ash (LTA). The detailed band assignments of coal spectra and the integration method of these FTIR bands were widely described elsewhere<sup>14,17</sup>. Selected indices derived from FTIR data using the integrated area (A) or the maximum intensity (H) of different spectral bands are described in Table 2.

### Statistical analyses.

The factor analysis used is based on the Principal Component Analysis or PCA (STATISTICA software, Statsoft Inc.). The principle of this multivariate statistical method<sup>18</sup> is to create new independent variables (*i. e.*, factors) that are the linear combination of original variables (*i. e.*, FTIR and SF indices) which are correlated to each other. The primary objective of the statistical analysis is to reduce the dimensionality of the data to a few important components or factors that best explain the variation in the data. From the data matrix, its standardized version Z and correlation matrix R were calculated. The correlation matrix R was used as a starting matrix in PCA. Principal components (PC) were determined by considering eigenvalues and associated eigenvectors. For plotting purpose only two or three PC scores were used. These must explain over 80% of the total variance. In R-mode factor analysis, the initial variables are scaled, thus the links between variables can be easily visualized. In Q-mode, the observations are scaled on the same set of factor axes. Coking coals with similar FTIR and SF index values are gathered in factor space and specific variables, which are important in distinguishing the different groups of coals, are determined.

## RESULTS AND DISCUSSIONS

The chemical characteristics of coals, before and after preheating, have been studied using FTIR and SF spectroscopies in order to determine (i) the structural modification occurring during preheating, (ii) the relationships between Reflectance and Volatile Matter (VM) amount, standing for thermal maturity reference parameters, and structural parameters, (iii) the chemical structures acting on plastic properties (Gieseler maximum fluidity, GI ; Arnu dilatation)<sup>10, 19</sup>.

As a matter of fact, the fluid properties (*i.e.* plastic properties) is an important step of coking because of the quality dependence of the semi-coke. However, fluidity leads to gas production increasing pressure inside the coke oven<sup>1</sup>. The optimization of the fluidity and the gas pressure becomes necessary. Moreover, preheating produces a decrease in the volatile matter content of the preheated coal compared to the original coal<sup>11</sup>. All those parameters could be maturity-/origin-dependent. To get coking performance related to structural parameters, Gieseler Index (maximum fluidity), Arnu (dilatation), Reflectance and Volatile Matter (maturity) were included in the statistical analysis.

The first step of this work was to characterize wet coking coals. Along this line, a first Principal Component Analysis was performed to relate chemical features to plastic properties as well as to visualize the main characteristics of the total sampling. The first PCA explains 87% of the total variance with 3 factors (Table 3). The factor 1 is related to the coking coal maturity with, in its positive way, a high reflectance value (*i.e.* REFLECT) and a low volatile matter amount (*i.e.* VM) (Figure 1a). This corresponds to a high aromatic structure amount in the residue (*i.e.* Aromatic H Index: H ARO and Aromatic/Aliphatic ratio : AH) and a high amount of highly polycondensed aromatics in the extract (predominance of 4-5 polycondensed aromatic rings compared to 2-3 rings, *i.e.* A3/A1). The factor 2 is characteristic, in its positive way, of an important dilatation of coal during coke making corresponding to a low branched aliphatic content in the residue (BA index). This PCA allows to classify three groups of coking coals. We can notice that the intermediate group shows the lowest expansion (Figure 1b). The third factor, representative of aliphatic structures within coking coal residues, underlines that the volatile matter amount (VM on factor 1) is independent of these structures (Figure 2).

A second PCA has been performed from spectroscopic data and plastic properties measured before and after preheating in order to know the chemical structures involved in coking property changes during preheating. This second PCA which explains 83% of the total variance with 3 factors (Table 4), underlines the main chemical changes during this step. The aromaticity of all the coals increases with a loss of aliphatic structures, in the residues (increase in Aromatic Index: AI and decrease in Factor of Aliphaticity: FA and in  $vCH_2$  asym/ $vCH_2$  sym: W) in spite of their maturity rank except for one coal which underwent a low evolution (i.e. T3595H). The fluidity and the volatile matter of coals, related to factor 1, slightly decrease during preheating except for T3614H (Figure 3). In its negative sense, the third factor concurrently underlines the loss of alkane side-chains on aromatic structures (i.e. SS1) in the residues and an increase in aromatic hydrogen content (i.e. H ARO) (Figure 4). Some coals act during preheating as described above (e.g. T3637H, T3614H, T3595H, T3591H). No changes are noted for aromatic structure substitutions of the other coals. This PCA underlines that the preheating mainly consists in an aromatization and thermodesorption, the chemical structures within the more mature coals changing less than the less mature ones. Consequently, coals have a slight difference in their properties after preheating.

Then, from those spectral data, multivariate linear regressions were performed to determine the relationships between structural characteristics, petrography parameters and plastic properties.

The first model was established to estimate the Reflectance from only three independent and standardized spectroscopic variables calculated from wet coals. The following equation was obtained :

$$Y_{\text{REFLECT}} = -0.59 X_{\text{H/C}} + 0.37 X_{\text{ACI}} + 0.68 X_{\text{A3/A1}} \quad (1)$$

The first model explains 96% of the total adjusted variance (adjusted  $r^2 = 0.96$ ), the standard error of the predicted value being 0.3. This model underlines an increase in maturity with the decrease in H/C ratio. The higher the maturity of coking coals, the higher their aromaticity in their residue and the higher their highly condensed aromatic content in their extract (Figure 5a).

Gas emission during coke making can also be evaluated by the volatile matter content in wet and preheated coals. Consequently, a second predictive model of the volatile matter amount was performed from structural indices measured before and after preheating (equation 2):

$$Y_{\text{V.M.}} = -0.63 X_{\text{BA}} - 0.34 X_{\text{H ARO}} - 0.22 X_{\text{ACI}} - 0.48 X_{\text{A3/A1}} \quad (2)$$

This model explains 85% of the total variance and the standard error of the predicted value is 2 (Figure 5b). Few changes in volatile matter amount is noted during preheating. This parameter inversely depends on the maturity (aromaticity of coking coals). The less aromatic the structures and/or the more substituted the aromatic structures within coal residues, the less polycondensed the aromatic structures within extracts, the more the volatile matter amount within coals. The V.M. also depends on the aliphatic nature in the residue because the volatile matter content inversely relates to the branched aliphatic index (i.e. BA).

Those two predictive models underline the relationships within coals between chemical structures, their reflectance and their volatile matter amount.

At last, one of the most important factors occurring on coke making has been predicted : the Gieseler Index, representing the maximum fluidity for coking coals. The optimal values of this index are between 500 and 1500 ddp<sup>m</sup>. To simplify, GI values have been expressed in log ddp<sup>m</sup>. Two models were established, one for wet coals and one for preheated coals (equations 3 and 4) because the predictive model of GI, after preheating, requires one more parameter which is the H/C ratio.

$$\text{For wet coals : } Y_{\text{GI}} = -0.84 X_{\text{BA}} + 0.61 X_{\text{SS1}} - 0.61 X_{\text{AH}} - 0.27 X_{\text{A3/A1}} \quad (3)$$

$$\text{For preheated coals : } Y_{\text{GI}} = 0.25 X_{\text{BA}} - 0.40 X_{\text{SS1}} - 0.74 X_{\text{AH}} - 0.34 X_{\text{A2/A1}} + 0.63 X_{\text{H/C}} \quad (4)$$

Those models respectively explain 95% and 97% of the total variance. In both cases, standard error of estimate is 0.2. Those models depend, in the coal residue, on the branched aliphatic ratio, the percentage of the highly substituted aromatic structures and the aromaticity (Figure 6). GI is inversely linked to the polycondensation of aromatic structures, in the coal extracts. However, even if trends are the same in coal extracts towards GI, before or after preheating, that is not the case in coal residues. Before preheating, the higher the maximum fluidity for coals, the more substituted the aromatic structures and the less branched the aliphatic structures. After preheating, one can observe the opposite relationships between the maximum fluidity, the aromatic substitution level and the branched aliphatic ratio. Furthermore, GI parameter decreases during preheating. Those results would underline the irreversible changes which occur in the organic matrix and pore structure of coal during preheating process and would explain the

different behaviors of the preheated coals during carbonization<sup>11, 20</sup>. As a matter of fact, preheated coals cannot be compared with wet coals because of the differences noted in the relationships between chemical structures and plastic properties.

## CONCLUSION

FTIR data on coal residues and SF data on coal extracts give complementary information. Coking coal chemical composition can be quantified from few spectroscopic indices. A ranking of coking coals from those data would be possible.

The main changes occurring during preheating are an aromatization with loss of alkane side-chains, in the solid residue for some coals, and a thermodesorption of the volatile compounds.

Principal Component Analysis showed the correlation between some structural indices and coal rank parameters, and the combined effects of some composition parameters on the plastic properties.

Some physical and plastic properties were predicted from few FTIR and SF indices of coking coals: Reflectance, the Volatile Matter amount and the Gieseler maximum fluidity.

Such investigations provide global as well as structural parameters that facilitate the understanding of the mechanisms involved during the different natural and industrial transformations of coals.

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Table 1 : Petrography and plastic properties of a series of ten coking coals, before and after preheating. These data have been given by INCAR-CSIC, Oviedo, Spain.

Origin	Coking coals: Wet (H) Preheated (P)	H atom/ C atom : H/C	Reflectance: REFLECT	Volatile Matter VM	Dilatation: ARNU	Maximum fluidity, Gieseler Index : GI
Australia	T3631H	0.720	1.41	19.5	70	1.68
Germany	T3637H	0.695	1.18	22.4	52	1.64
Australia	T3622H	0.751	1.09	23.2	75	3.17
USA	T3639H	0.683	1.15	24.2	123	2.50
Spain	T3595H	0.726	1.25	25.6	171	3.99
Poland	T3625H	0.728	1.00	28.5	147	2.59
USA	T3658H	0.760	1.00	30.8	279	4.25
Spain	T3590H	0.720	0.96	31.4	218	4.00
USA	T3614H	0.750	0.90	33.8	143	4.01
Spain	T3591H	0.760	0.84	35.9	135	4.03
Australia	T3631P	0.669		20.4	33	0.78
Germany	T3637P	0.694		22.3	42	0.90
Australia	T3622P	0.732		23.4	66	2.57
USA	T3639P	0.713		24.1	109	2.02
Spain	T3595P	0.756		24.0	134	3.16
Poland	T3625P	0.753		28.1	88	2.60
USA	T3658P	0.763		30.6	273	3.90
Spain	T3590P	0.692		32.1	177	3.37
USA	T3614P	0.746		33.6	137	3.67
Spain	T3591P	0.724		35.8	101	3.43

Table 2 : FTIR and SF indices calculated from spectral data measured for each coking coal. A:

Area, H : Height. For FTIR data, the subscript number of Area (e.g. A<sub>3050</sub>) represents the wavenumber (cm<sup>-1</sup>) at the top of the spectral band, integrated from valley to valley. The subscript number of Height (e.g. H<sub>1600</sub>) represents the wavenumber (cm<sup>-1</sup>) at the top of the band at which the height is measured. For SF data, the two subscript numbers represent the area band limits (nm), used to measure the absolute value of the fluorescence emission. These indices and their significance have been well described by Kister *et al.*<sup>14</sup>

Indices calculated from :	From FTIR spectra							From SF spectra	
	H ARO A <sub>3050</sub> / A <sub>2920</sub>	W H <sub>2920</sub> / H <sub>2855</sub>	BA H <sub>1380</sub> / H <sub>1440</sub>	ACI H <sub>1600</sub> / (H <sub>1440</sub> + H <sub>1440</sub> )	FA (H <sub>2920</sub> +H <sub>2850</sub> )/ (H <sub>1600</sub> +H <sub>2920</sub> + H <sub>2850</sub> )	SSI A <sub>864</sub> / A <sub>864+743</sub>	AH A <sub>864-743</sub> / A <sub>2920</sub>	A2/A1 A <sub>460-370</sub> / A <sub>370-300</sub>	A3/A1 A <sub>580-460</sub> / A <sub>370-300</sub>
T3631H	0.142	1.675	0.807	0.586	0.472	0.186	0.941	3.46	0.936
T3637H	0.108	1.695	0.850	0.511	0.504	0.201	0.811	2.85	0.667
T3622H	0.113	1.646	0.826	0.577	0.481	0.204	0.809	2.44	0.600
T3639H	0.176	1.733	0.799	0.533	0.504	0.185	0.919	2.62	0.568
T3595H	0.163	1.684	0.771	0.573	0.475	0.214	0.917	2.98	0.832
T3625H	0.113	1.692	0.807	0.519	0.491	0.182	0.863	2.55	0.604
T3658H	0.102	1.800	0.791	0.596	0.491	0.170	0.697	2.49	0.528
T3590H	0.115	1.708	0.767	0.523	0.517	0.170	0.734	2.73	0.767
T3614H	0.107	1.681	0.796	0.568	0.474	0.194	0.772	2.19	0.444
T3591H	0.091	1.667	0.779	0.566	0.457	0.154	0.713	1.82	0.308
T3631P	0.149	1.565	0.796	0.623	0.444	0.226	1.033	3.61	0.819
T3637P	0.177	1.671	0.852	0.572	0.430	0.178	1.174	2.41	0.394
T3622P	0.114	1.613	0.839	0.582	0.429	0.180	1.051	2.29	0.408
T3639P	0.190	1.657	0.806	0.550	0.474	0.173	1.044	2.92	0.571
T3595P	0.164	1.597	0.788	0.586	0.480	0.207	0.930	3.13	0.727
T3625P	0.122	1.619	0.816	0.501	0.447	0.208	0.958	2.48	0.482
T3658P	0.118	1.706	0.801	0.585	0.462	0.201	0.778	2.32	0.374
T3590P	0.126	1.626	0.804	0.543	0.465	0.166	0.809	3.20	0.706
T3614P	0.097	1.627	0.771	0.577	0.457	0.171	0.848	2.70	0.472
T3591P	0.101	1.623	0.773	0.576	0.425	0.136	0.788	1.87	0.318

Table 3 : Results of the first PCA performed from wet coal data. 9 variables (V.M., ARNU, REFLECT, H ARO, AH, BA, W, FA and A3/A1) were selected for 10 coking coals. 3 factors were extracted and explain 87 % of the total variance.

Factor	Eigenvalues	% total variance	Cumul. Eigenval.	Cumul. % total variance
1	4.4	49	4.4	49
2	2.1	23	6.5	72
3	1.3	15	7.8	87

Table 4 : Results of the second PCA performed from wet and preheated coal data. 9 variables (V.M., GI, H ARO, ACI, AH, BA, W, FA and SSI) were selected for 20 coking coals. 3 factors were extracted and explain 83 % of the total variance.

Factor	Eigenvalues	% total variance	Cumul. Eigenval.	Cumul. % total variance
1	4.0	44	4.0	44
2	2.3	26	6.3	70
3	1.2	14	7.5	83

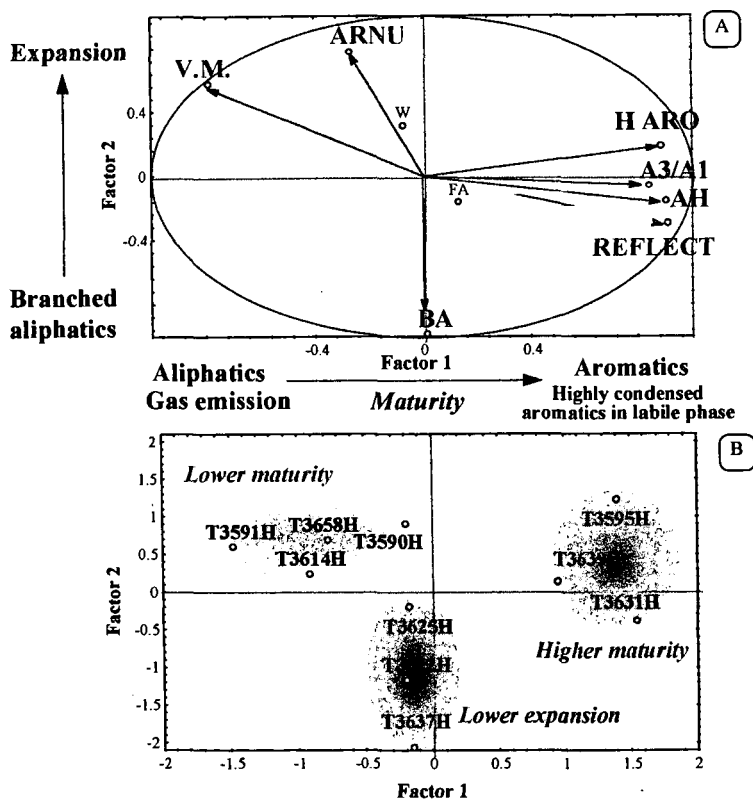


Figure 1 : First PCA performed from 9 variables (spectroscopic indices, petrography and plastic properties) and 10 wet coking coals. This PCA explains 87% of the total variance with 3 factors. This figure shows the 2 first Principal Components (PC) and visualizes the main chemical and physical characteristics of wet coals. A/ R-mode factor analysis : initial variables. B/ Q-mode factor analysis : coking coals.

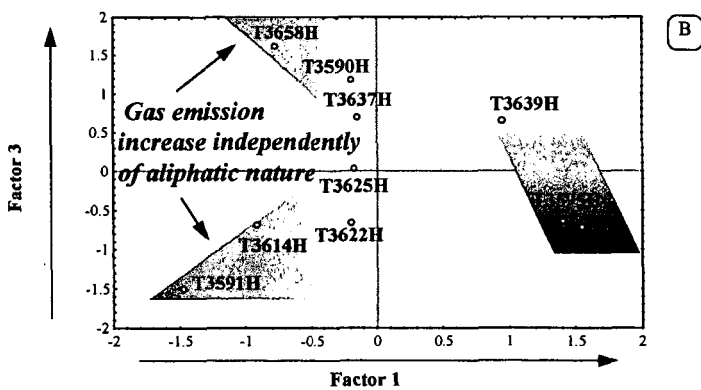
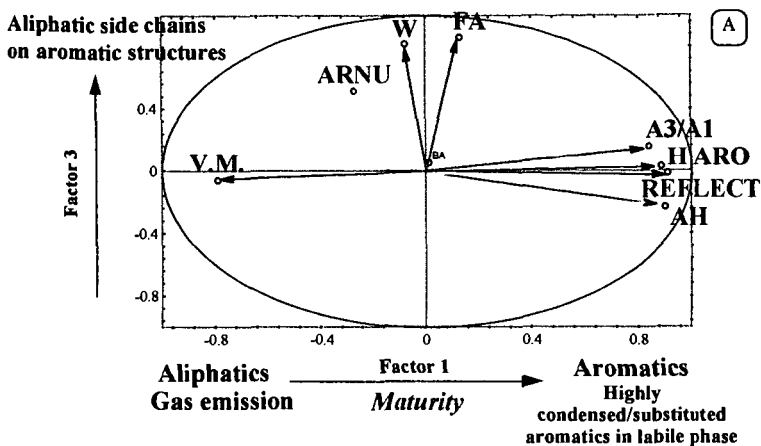


Figure 2 : First PCA performed from 9 variables (spectroscopic indices, petrography and plastic properties) and 10 wet coking coals. This PCA explains 87% of the total variance with 3 factors. This figure shows the 2nd and the 3rd Principal Components (PC). A/ R-mode factor analysis : initial variables. B/ Q-mode factor analysis : coking coals.

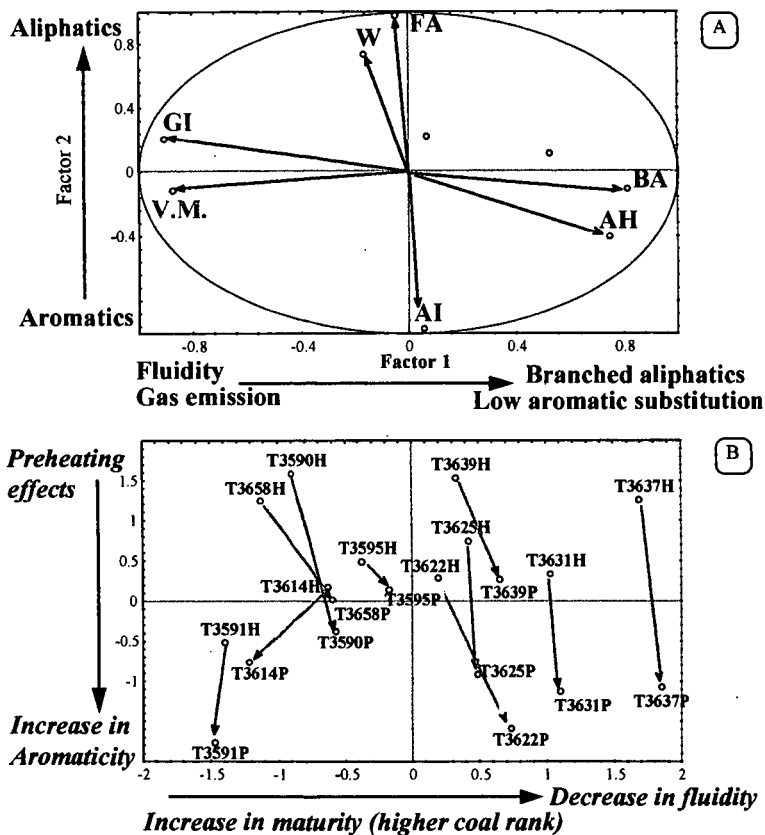


Figure 3 : Comparison between plastic property and structural characteristics changes during preheating. Second PCA performed from 9 variables (spectroscopic indices, petrography and plastic properties) and 20 (wet and preheated) coking coals. This PCA explains 83% of the total variance with 3 factors. This figure shows the 1st and the 2nd Principal Components (PC). A/ R-mode factor analysis : initial variables. B/ Q-mode factor analysis : coking coals.



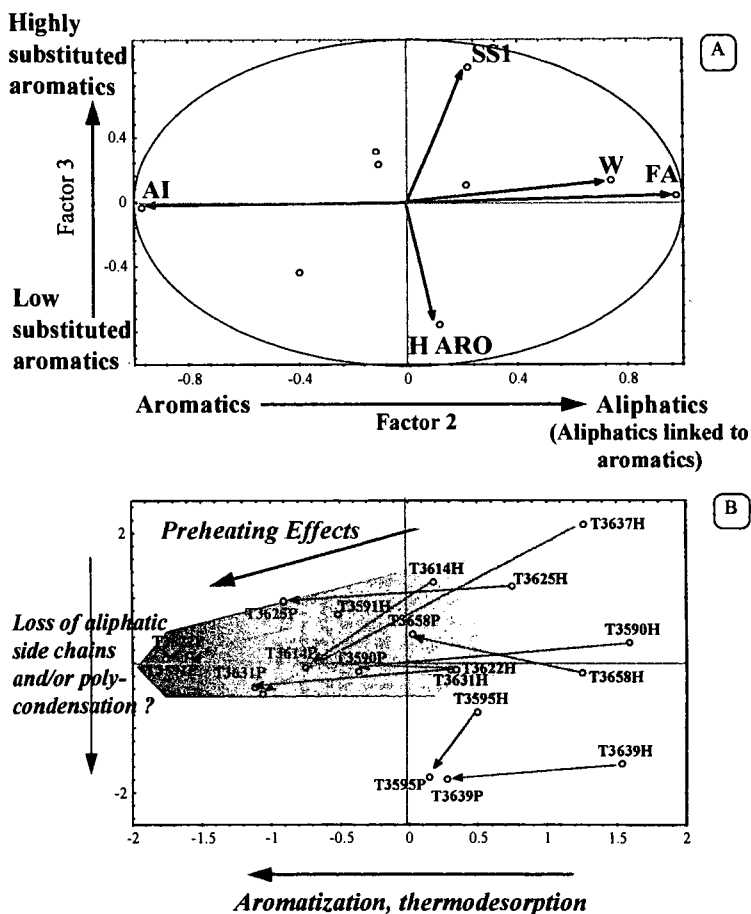


Figure 4 : Aromatic changes during preheating. Second PCA performed from 9 variables (spectroscopic indices, petrography and plastic properties) and 20 (wet and preheated) coking coals. This PCA explains 83% of the total variance with 3 factors. This figure shows the 2nd and the 3rd Principal Components (PC). A/ R-mode factor analysis : initial variables. B/ Q-mode factor analysis : coking coals.

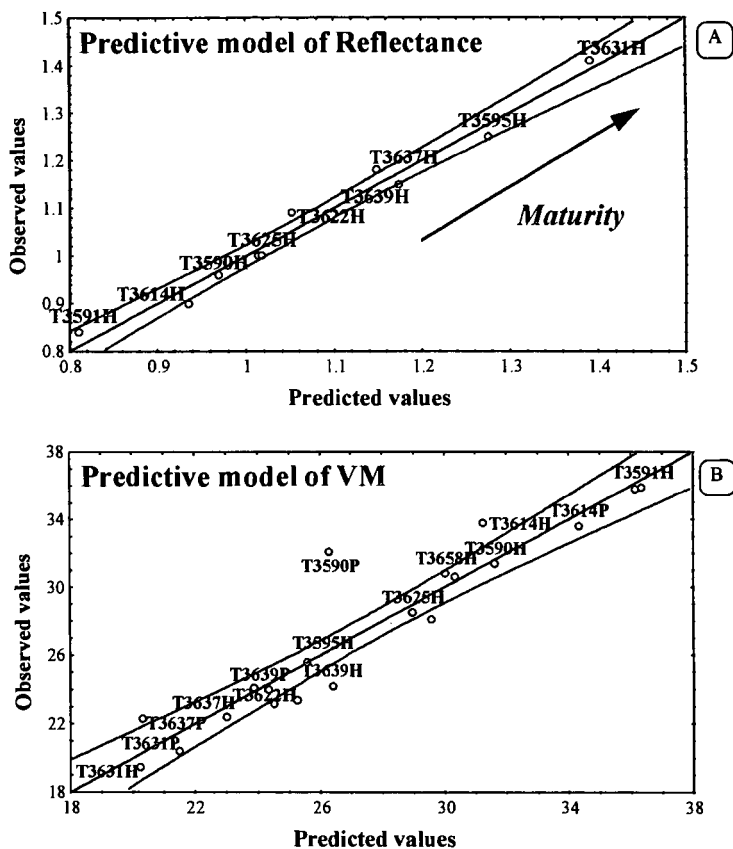


Figure 5: Prediction of the petrography properties of the coking coals by Multivariate Linear Regression (MLR) A/ Predictive model of Reflectance from wet coal data (3 indices, 10 coals, Adjusted  $R^2 = 0.96$ ,  $F(3,6)=79$ ,  $p<0.00003$ , Std. Error of estimate: 0.03). B/ Predictive model of Volatile Matter Amount (VM) from wet and preheated coal data (4 indices, 20 coals, Adjusted  $R^2 = 0.85$ ,  $F(4,15)=28$ ,  $p<0.00000$ , Std. Error of estimate: 2).

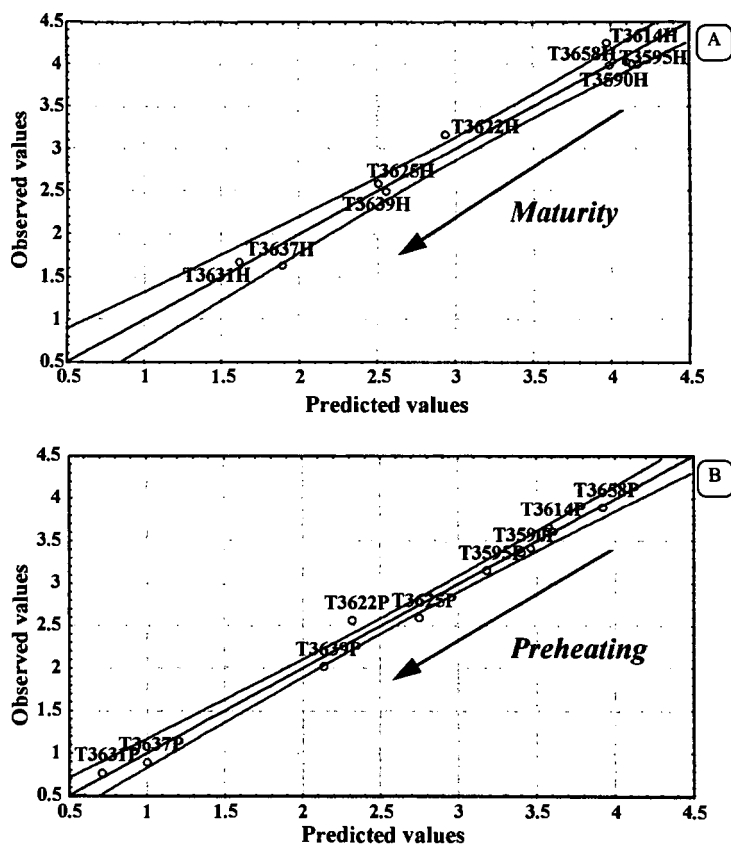


Figure 6: Prediction of the plastic properties of the coking coals by Multivariate Linear Regression (MLR) A/ Predictive model of Gieseler Index (GI from wet coal data (4 indices, 10 coals, Adjusted  $R^2 = 0.95$ ,  $F(5,4)=44$ ,  $p<0.0004$ , Std. Error of estimate: 0.2). B/ Predictive model of GI from preheated coal data (5 indices, 10 coals, Adjusted  $R^2 = 0.97$ ,  $F(5,4)=70$ ,  $p<0.0006$ , Std. Error of estimate: 0.2).